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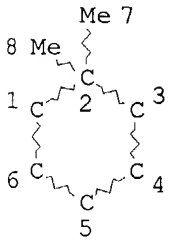
L12 STR



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DEFAULT ECLEVEL IS LIMITED

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NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
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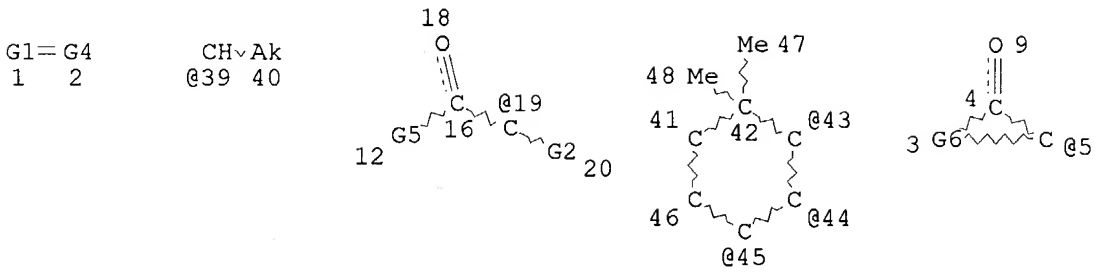

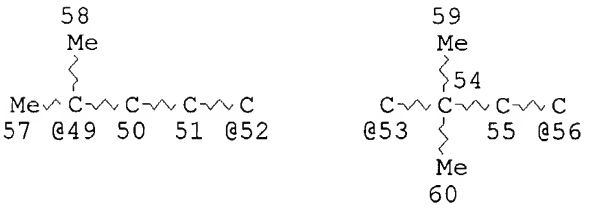

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VAR G2=H/ME
VAR G4=CH2/39
VAR G5=43/44/45
VAR G6=49-4 52-5/52-4 49-5/53-4 56-5/56-4 53-5
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 33

STEREO ATTRIBUTES: NONE
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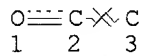
L20 398 SEA FILE=REGISTRY SUB=L18 SSS FUL L12 AND L16
L21 317 SEA FILE=HCAPLUS ABB=ON PLU=ON L20(L)PREP/RL
L28 TRANSFER PLU=ON L21 1- RN : 5326 TERMS
L29 5326 SEA FILE=REGISTRY ABB=ON PLU=ON L28
L30 STR



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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
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STEREO ATTRIBUTES: NONE
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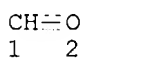
L33 STR



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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 2

STEREO ATTRIBUTES: NONE
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L36 280202 SEA FILE=HCAPLUS ABB=ON PLU=ON L32(L)(RACT OR RCT OR RGT)/RL

L37 114368 SEA FILE=HCAPLUS ABB=ON PLU=ON L35(L)(RACT OR RCT OR RGT)/RL

L38 98133 SEA FILE=HCAPLUS ABB=ON PLU=ON L36 AND L37
L39 111 SEA FILE=HCAPLUS ABB=ON PLU=ON L38 AND L21
L40 4 SEA FILE=REGISTRY ABB=ON PLU=ON L29 AND (TI OR ZR OR HF)/ELS

L41 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L39 AND L40

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L41 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:906114 HCAPLUS
DOCUMENT NUMBER: 138:4201
TITLE: Catalytic system for aldol reactions
INVENTOR(S): Jacoby, Denis
PATENT ASSIGNEE(S): Firmenich Sa, Switz.
SOURCE: PCT Int. Appl., 19 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002094755	A1	20021128	WO 2002-IB1839	20020521
W: CN, IL, IN, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
EP 1395542	A1	20040310	EP 2002-730616	20020521
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
US 2004082818	A1	20040429	US 2003-688297	20031017

PRIORITY APPLN. INFO.: WO 2001-IB902 W 20010522
WO 2002-IB1839 W 20020521

OTHER SOURCE(S): CASREACT 138:4201; MARPAT 138:4201

AB The invention relates to a process for the preparation, in a single step, of enones by an aldol condensation of a ketone, such as a gem-dimethylcyclohexylethanone or gem-dimethylcyclohexenylethanone derivative, with an aldehyde in the presence of a novel catalytic system and without the pre-formation of an enolate. Said catalytic system consists of a metal complex, such as a [(Cl)n(alkoxy)4-nTi] or [(Cl)n(alkoxy)4-nZr] complex (n = 1-3), and a co-ingredient, such as a carboxylic acid anhydride or an anhydrous salt. Thus, 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-1-ethanone was treated with MeCHO in presence of Zr(OPr)Cl3 and MgCl2 to give 45% 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-2-buten-1-one.

IC ICM C07C045-72
ICS C07C049-557; B01J031-12

CC 21-2 (General Organic Chemistry)

IT 106-31-0, Butyric anhydride 108-24-7, Acetic anhydride 123-62-6, Propionic anhydride **3981-83-7**, Isopropoxytitanium trichloride 7637-07-2, Boron trifluoride, uses 7705-08-0, Iron(III) chloride, uses 7757-82-6, Sodium sulfate, uses 7778-80-5, Potassium sulfate, uses 7786-30-3, Magnesium chloride, uses **31676-28-5**, Dipropoxyzirconium dichloride **113133-11-2**
RL: CAT (Catalyst use); USES (Uses)
(catalytic system for aldol reactions)

IT **71048-82-3P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(catalytic system for aldol reactions)

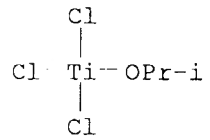
IT **50-00-0**, Formaldehyde, reactions **75-07-0**, Acetaldehyde, reactions **78-93-3**, 2-Butanone, reactions **107-02-8**, 2-Propenal, reactions **830-13-7**, Cyclododecanone **1193-47-1**, 2,2-Dimethylcyclohexanone **1197-92-8** **4170-30-3**, 2-Butenal **37709-66-3** **41435-93-2** **41436-46-8** **54201-08-0** **55981-43-6** **73956-68-0** **91819-58-8** **476689-60-8** **476689-61-9** **476689-64-2** **476689-65-3**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(catalytic system for aldol reactions)

IT 565-62-8P **23696-85-7P** **57020-37-8P** 65113-95-3P **83218-16-0P** **255058-92-5P** 344296-64-6P **476689-62-0P** 476689-63-1P

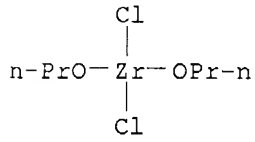
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(catalytic system for aldol reactions)

IT **3981-83-7**, Isopropoxytitanium trichloride **31676-28-5**, Dipropoxyzirconium dichloride **113133-11-2**
RL: CAT (Catalyst use); USES (Uses)
(catalytic system for aldol reactions)

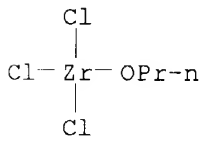
RN 3981-83-7 HCAPLUS
CN Titanium, trichloro(2-propanolato)-, (T-4)- (9CI) (CA INDEX NAME)



RN 31676-28-5 HCAPLUS
CN Zirconium, dichlorodipropoxy-, (T-4)- (9CI) (CA INDEX NAME)



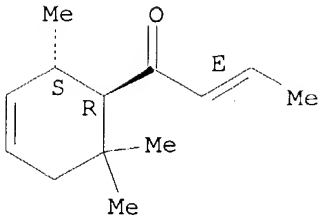
RN 113133-11-2 HCAPLUS
CN Zirconium, trichloropropoxy-, (T-4)- (9CI) (CA INDEX NAME)



IT **71048-82-3P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(catalytic system for aldol reactions)

RN 71048-82-3 HCAPLUS
CN 2-Buten-1-one, 1-[(1R,2S)-2,6,6-trimethyl-3-cyclohexen-1-yl]-, (2E)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



IT **50-00-0**, Formaldehyde, reactions **75-07-0**, Acetaldehyde, reactions **78-93-3**, 2-Butanone, reactions **107-02-8**, 2-Propenal, reactions **830-13-7**, Cyclododecanone **1193-47-1**, 2,2-Dimethylcyclohexanone **1197-92-8** **4170-30-3**, 2-Butenal **37709-66-3** **41435-93-2** **41436-46-8** **54201-08-0** **55981-43-6** **73956-68-0** **91819-58-8** **476689-60-8** **476689-61-9** **476689-64-2** **476689-65-3**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(catalytic system for aldol reactions)

RN 50-00-0 HCAPLUS
CN Formaldehyde (8CI, 9CI) (CA INDEX NAME)

$H_2C{=}O$

RN 75-07-0 HCAPLUS
CN Acetaldehyde (8CI, 9CI) (CA INDEX NAME)

$H_3C{-}CH{=}O$

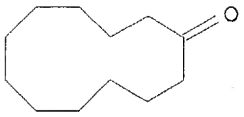
RN 78-93-3 HCAPLUS
CN 2-Butanone (8CI, 9CI) (CA INDEX NAME)

$H_3C{-}\overset{\overset{O}{\|}}{C}{-}CH_2{-}CH_3$

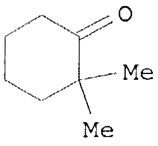
RN 107-02-8 HCAPLUS
CN 2-Propenal (9CI) (CA INDEX NAME)

$H_2C{=}CH{-}CH{=}O$

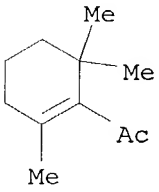
RN 830-13-7 HCAPLUS
CN Cyclododecanone (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



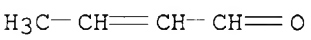
RN 1193-47-1 HCAPLUS
CN Cyclohexanone, 2,2-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



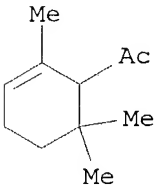
RN 1197-92-8 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



RN 4170-30-3 HCAPLUS
CN 2-Butenal (9CI) (CA INDEX NAME)

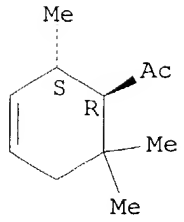


RN 37709-66-3 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



RN 41435-93-2 HCAPLUS
CN Ethanone, 1-[(1R,2S)-2,6,6-trimethyl-3-cyclohexen-1-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 41436-46-8 HCAPLUS
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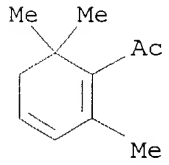
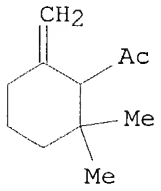
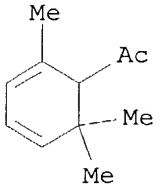


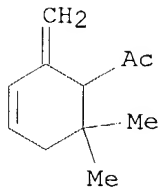
RN 54201-08-0 HCAPLUS
CN Ethanone, 1-(2,2-dimethyl-6-methylenecyclohexyl)- (9CI) (CA INDEX NAME)



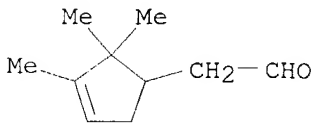
RN 55981-43-6 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-2,4-cyclohexadien-1-yl)- (9CI) (CA INDEX NAME)



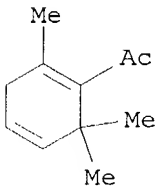
RN 73956-68-0 HCAPLUS
CN Ethanone, 1-(6,6-dimethyl-2-methylene-3-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



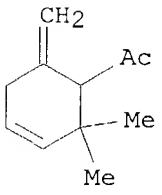
RN 91819-58-8 HCAPLUS
CN 3-Cyclopentene-1-acetaldehyde, 2,2,3-trimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



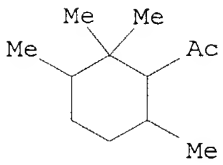
RN 476689-60-8 HCAPLUS
CN Ethanone, 1-(2,6,6-trimethyl-1,4-cyclohexadien-1-yl)- (9CI) (CA INDEX NAME)



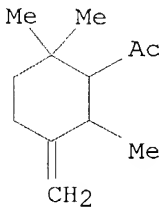
RN 476689-61-9 HCAPLUS
CN Ethanone, 1-(2,2-dimethyl-6-methylene-3-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



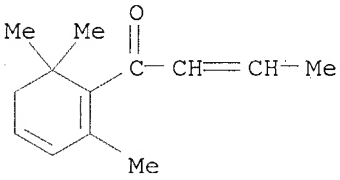
RN 476689-64-2 HCAPLUS
CN Ethanone, 1-(2,2,3,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)



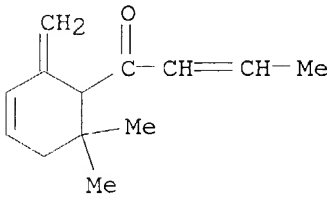
RN 476689-65-3 HCAPLUS
CN Ethanone, 1-(2,2,6-trimethyl-5-methylenecyclohexyl)- (9CI) (CA INDEX NAME)



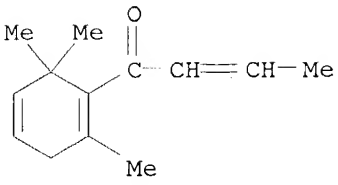
IT **23696-85-7P 57020-37-8P 83218-16-0P**
255058-92-5P 476689-62-0P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(catalytic system for aldol reactions)
RN 23696-85-7 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)- (8CI, 9CI) (CA INDEX NAME)



RN 57020-37-8 HCAPLUS
CN 2-Buten-1-one, 1-(6,6-dimethyl-2-methylene-3-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



RN 83218-16-0 HCAPLUS
CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1,4-cyclohexadien-1-yl)- (9CI) (CA INDEX NAME)



RN 255058-92-5 HCAPLUS
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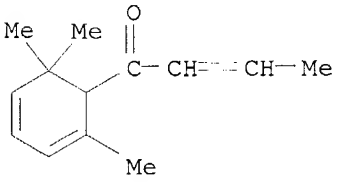

RN 476689-62-0 HCAPLUS
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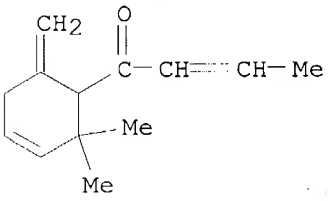

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT